

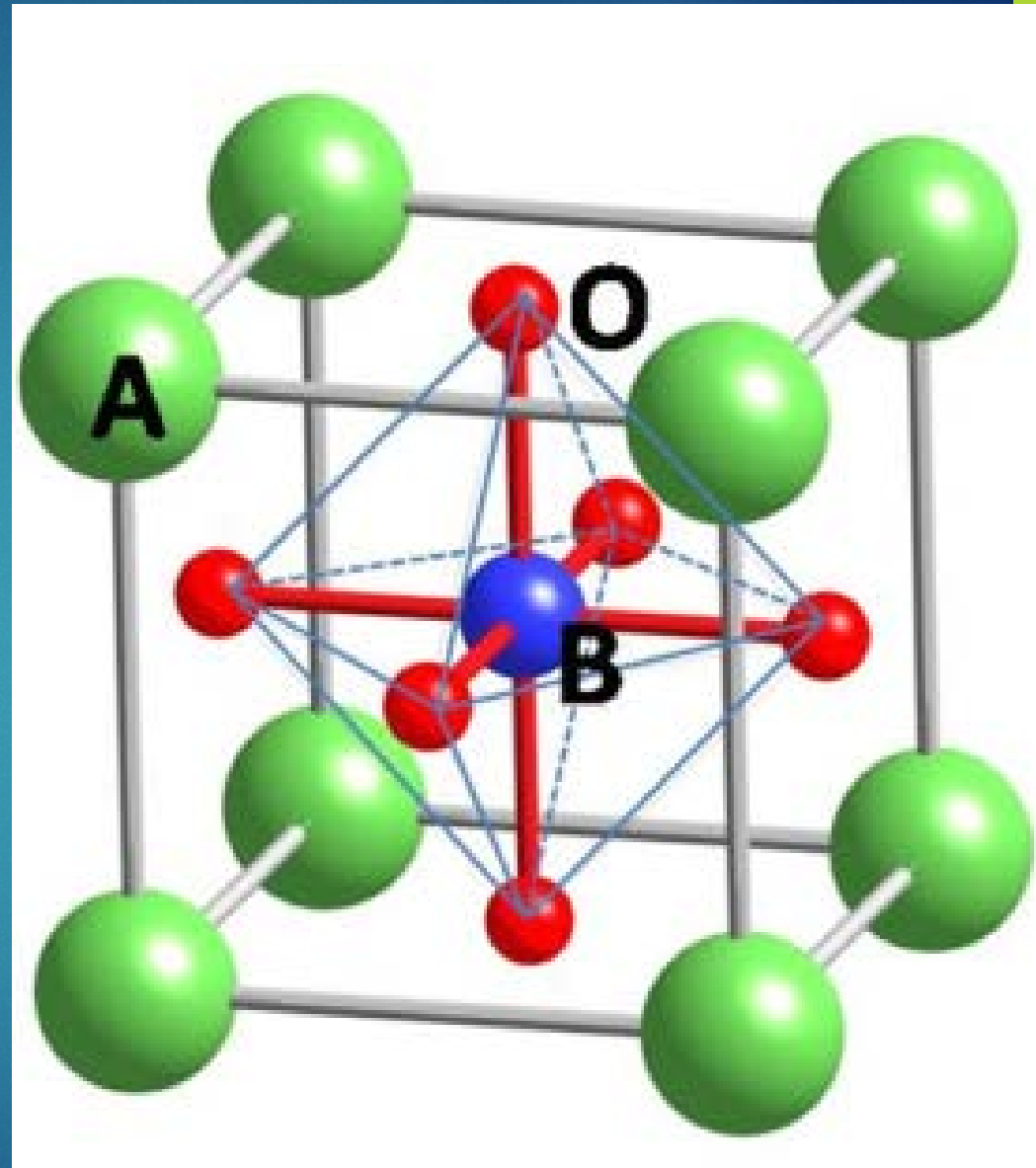
Visualization of Perovskite Octahedral Tilts in Augmented Reality

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MENTOR – WILLIAM RATCLIFF

Background

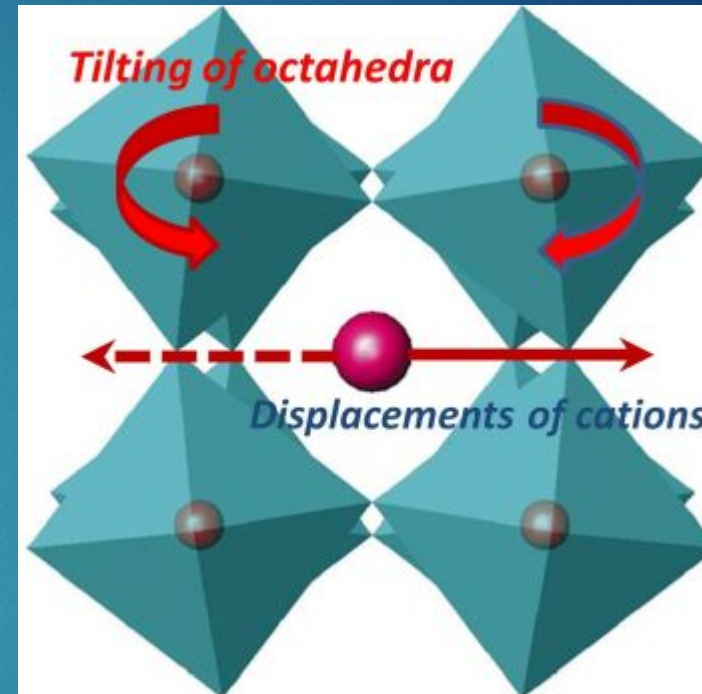
- ▶ Perovskites
 - ▶ Crystals with ABX_3 structure
 - ▶ X – anion
 - ▶ A – cation
 - ▶ B – cation



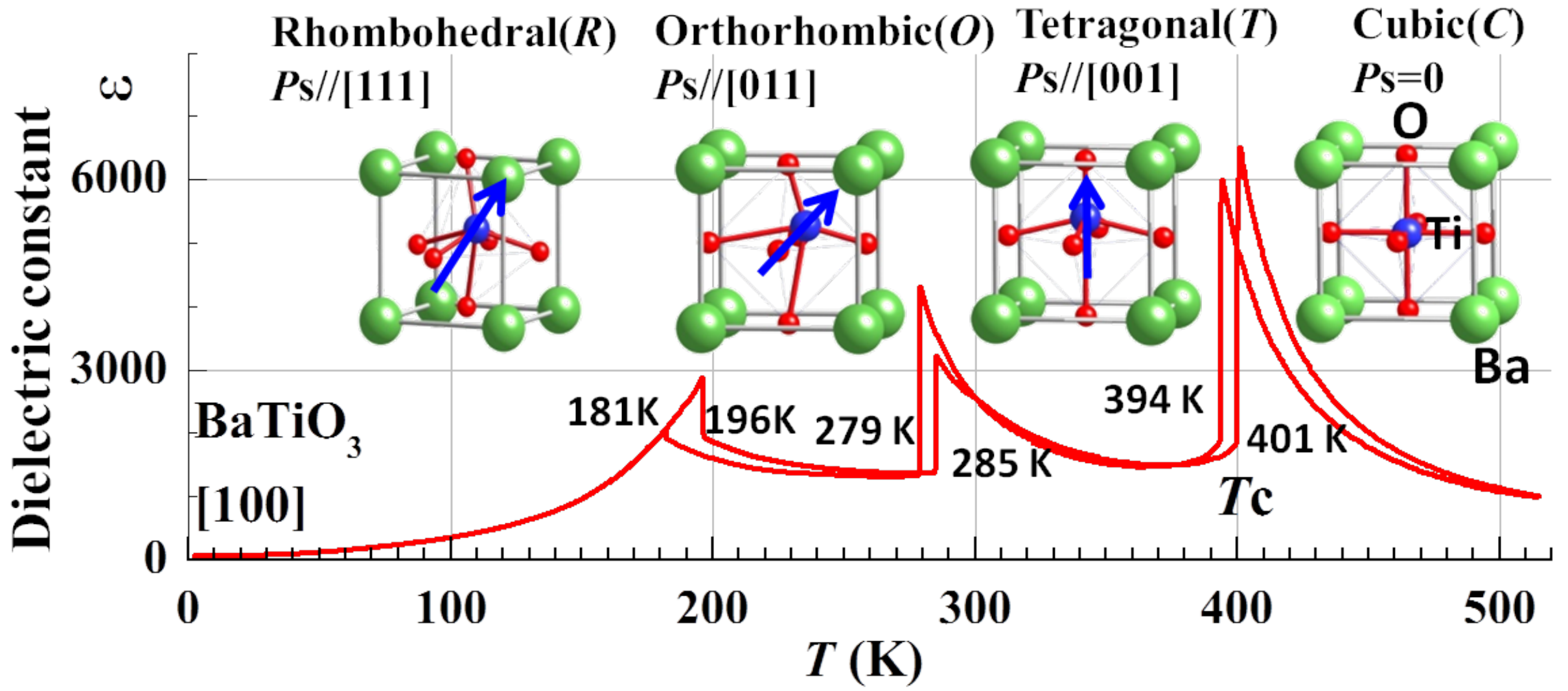
Perovskite Unit Cell (Courtesy of Fu and Itoh)

Crystal Distortions

- ▶ Distortions
 - ▶ Jahn-Teller Distortion
 - ▶ Cation Displacements
 - ▶ **Octahedral Tilts**
- ▶ Causes
 - ▶ Size of A and B ions
 - ▶ State Variables



Courtesy of Dr. Gorman

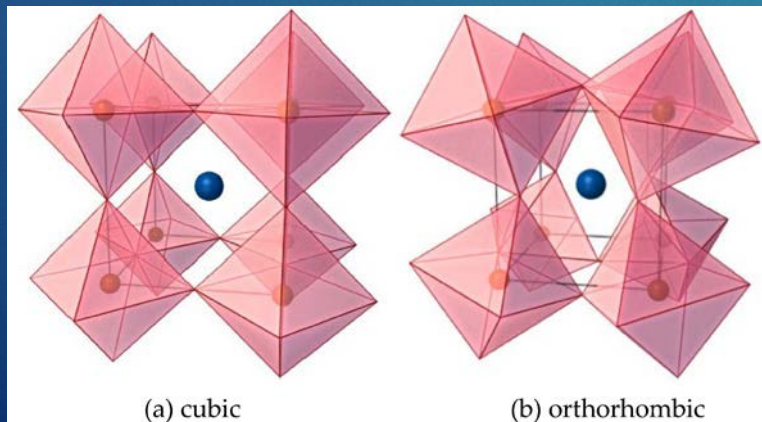


Cation Size

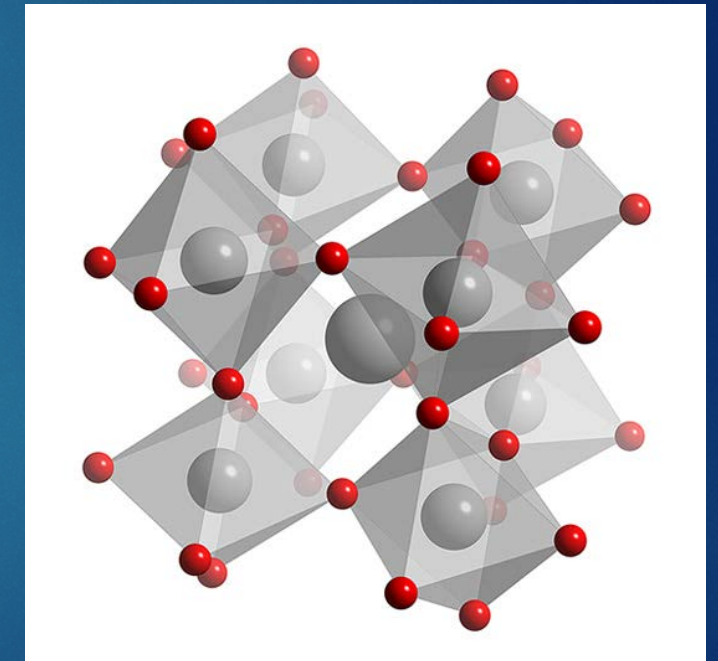
- ▶ Goldschmidt's tolerance factor (t) - ratio of A and B ionic radii that describe stability

$$t = \frac{r_A + r_O}{\sqrt{2}(r_B + r_O)}$$

- ▶ >1 = A ion too big or B ion too small = hexagonal
- ▶ $0.9 - 1$ = A and B ions are ideal = cubic
- ▶ $0.71 - 0.9$ = A ion too small = Orthorhombic/Rhombohedral



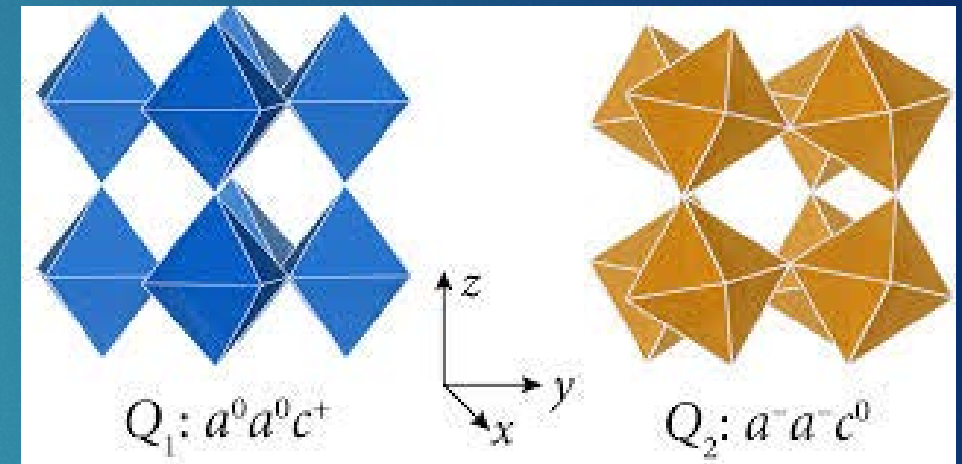
Courtesy of Mark Levy



CaTiO_3 Courtesy of Nick Greeves

Glazer Notation

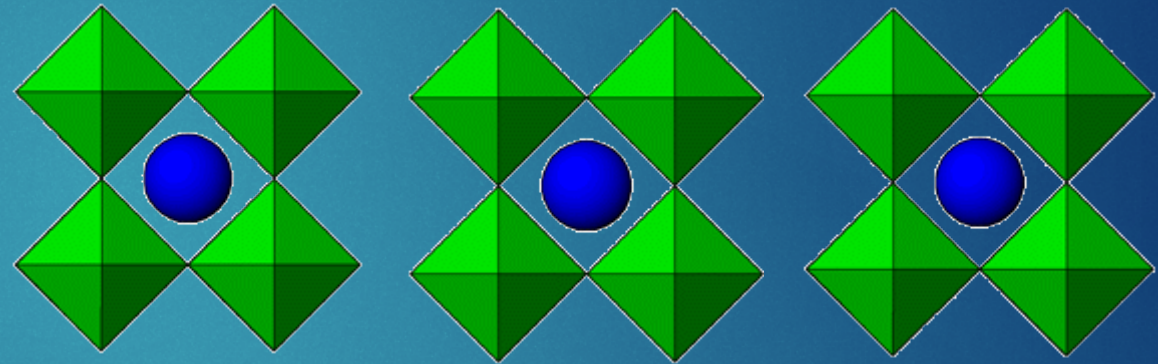
- ▶ Describe octahedral distortion
 - ▶ Sequence of symbols – axes
 - ▶ $a, a, a - x, y, z$
 - ▶ Identical characters – relative magnitude
 - ▶ a, a, c
 - ▶ Superscript – phase of tilt for layers
 - ▶ 0 = no
 - ▶ + = in phase
 - ▶ - = anti phase



Courtesy of Rondinelli and Fennie

Project Goal

- ▶ Improve visualization of Perovskite distortions by working in Augmented Reality
- ▶ 3D modeling programs
 - ▶ VESTA
 - ▶ SPuDS
 - ▶ Diamond



Courtesy of SPuDS

Unity3D



Courtesy of Guido Henkel

- ▶ Game engine for developing video games
- ▶ Language –Javascript/UnityScript, C#, Boo
- ▶ Deployment to VR/AR
 - ▶ Gear VR (phones)
 - ▶ HTC Vive
 - ▶ Oculus Rift
 - ▶ Windows Hololens



Courtesy of Wired



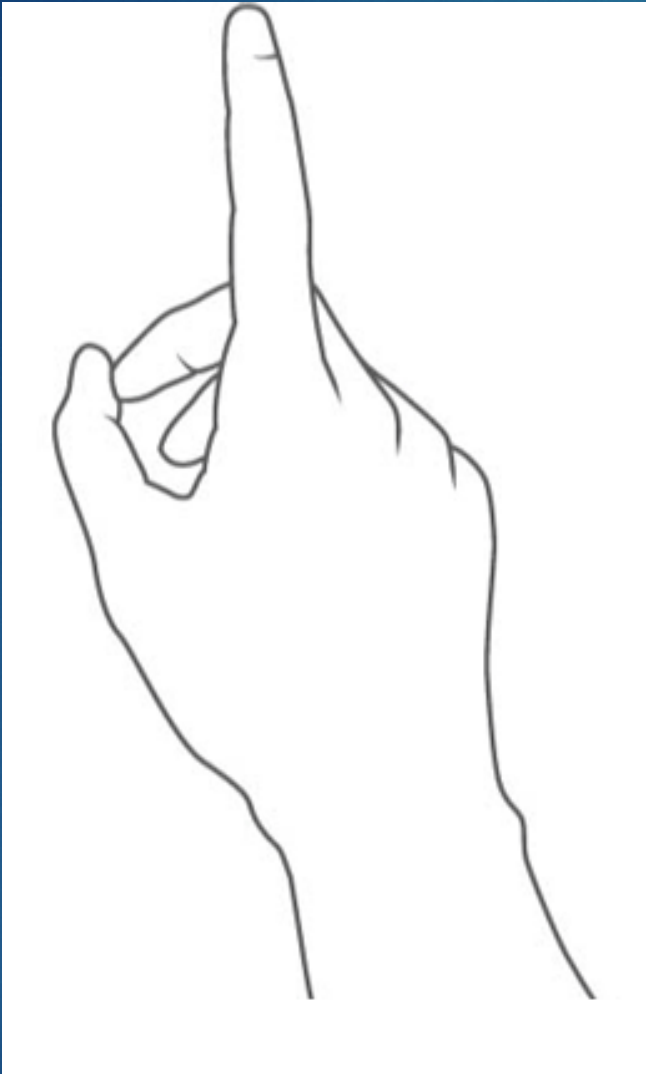
Courtesy of Microsoft

Microsoft Hololens

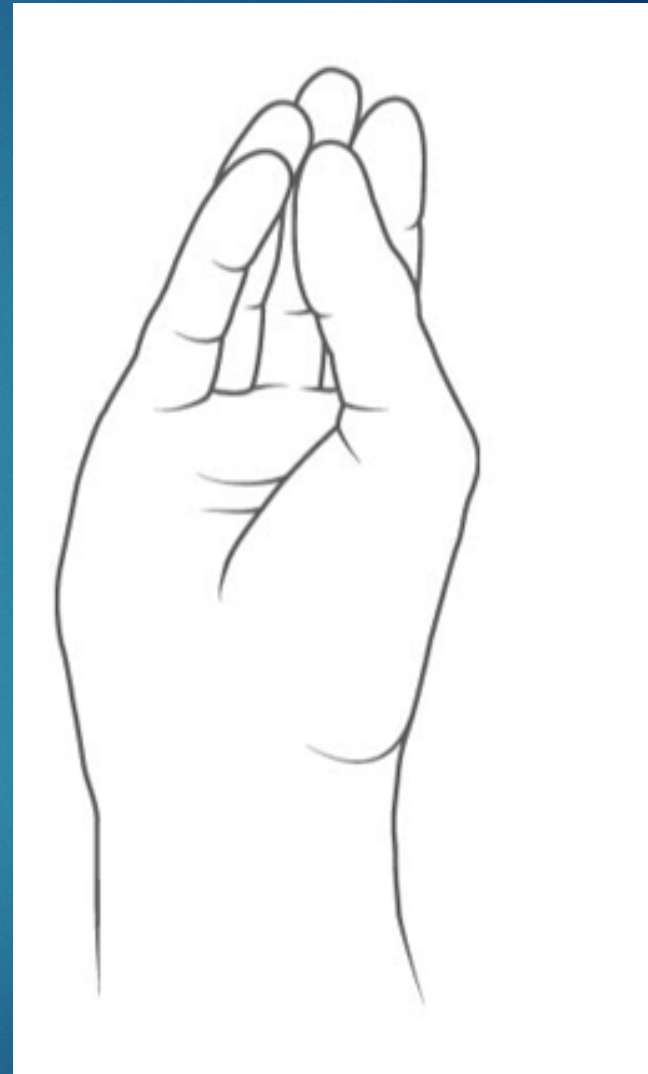
- ▶ Augmented Reality
- ▶ Spatial mapping, gesture/speech/gaze recognition



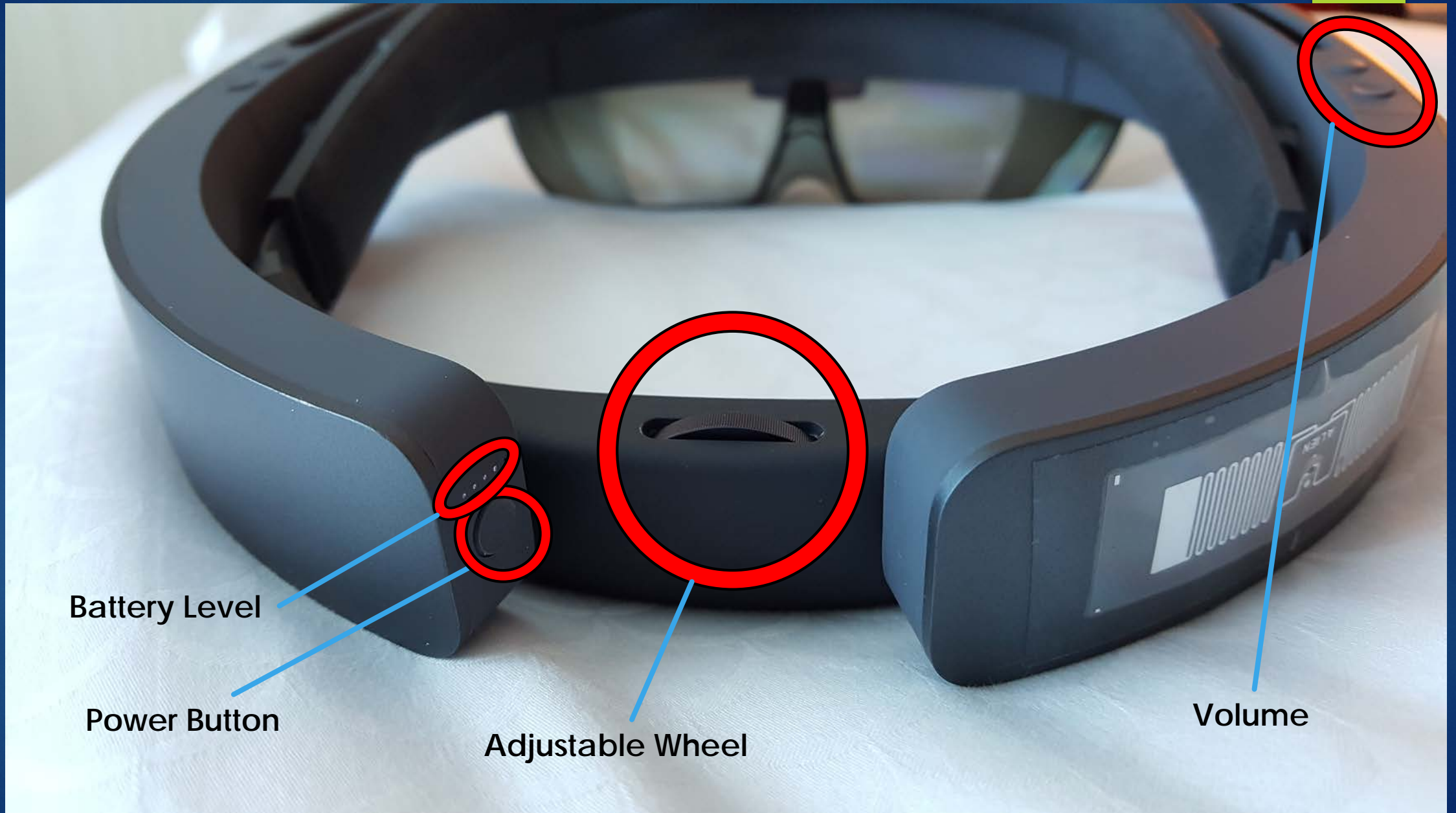
Courtesy of Forbes



Tap (Courtesy of Microsoft)



Bloom (Courtesy of Microsoft)



Battery Level

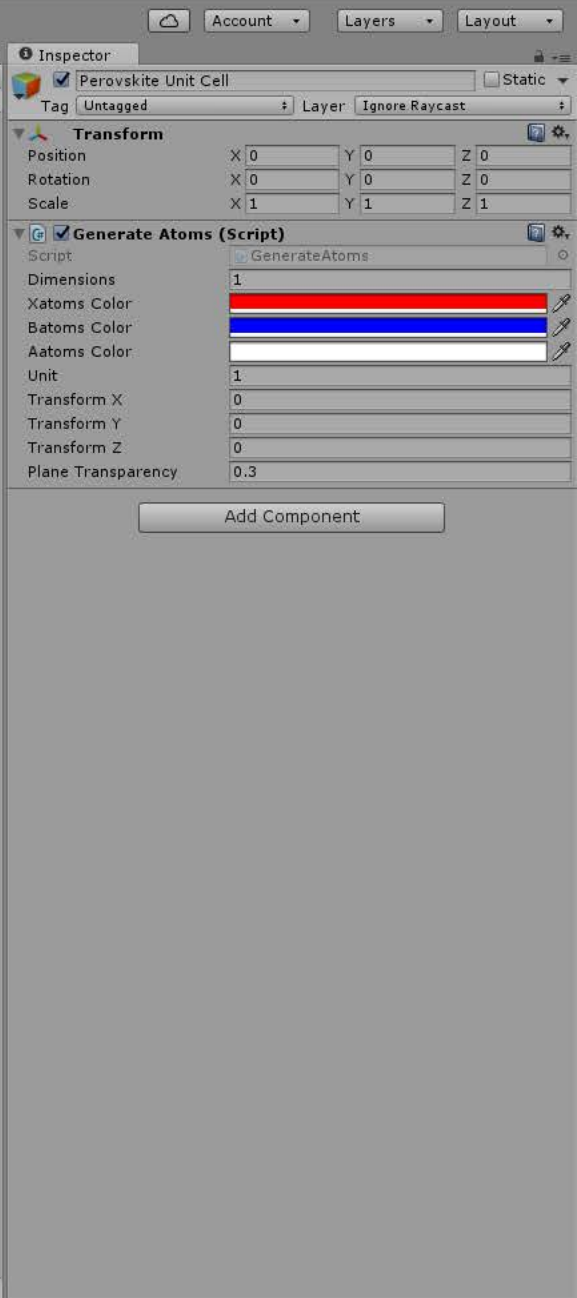
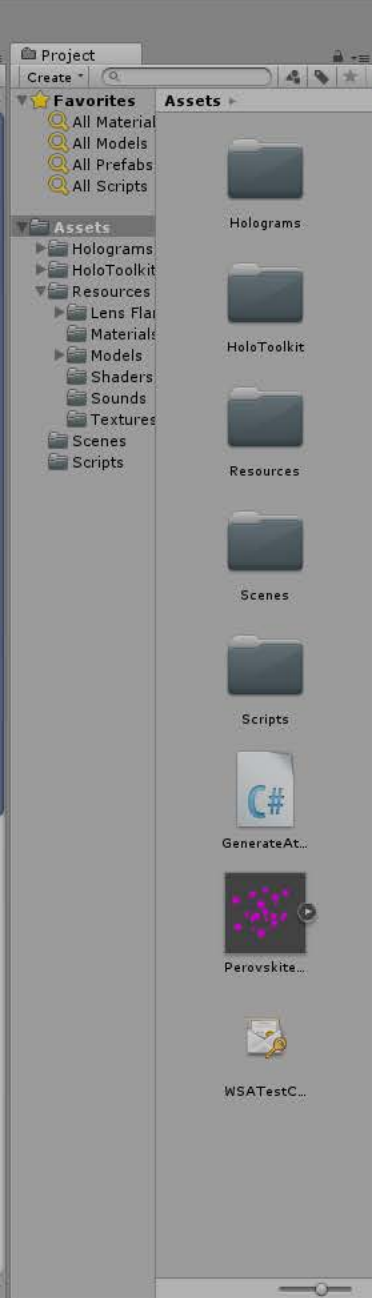
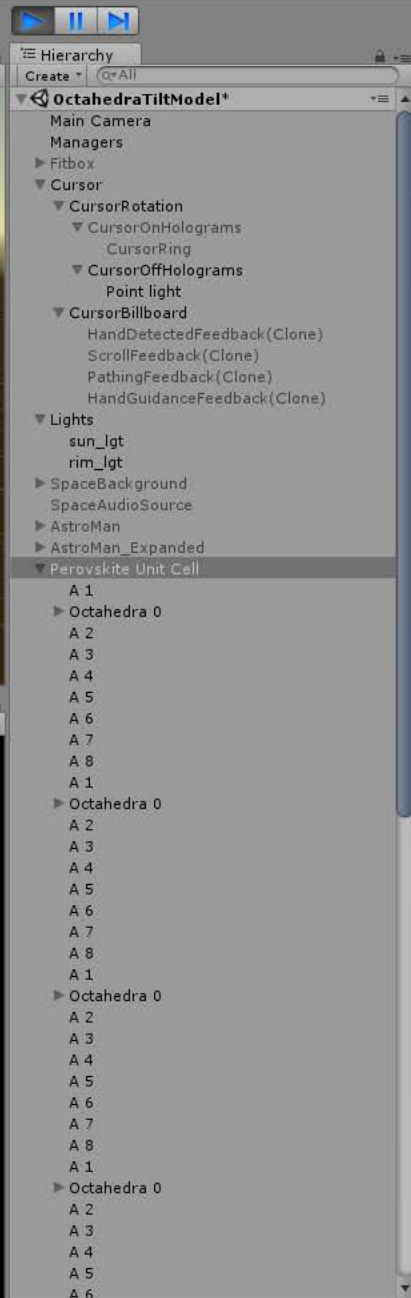
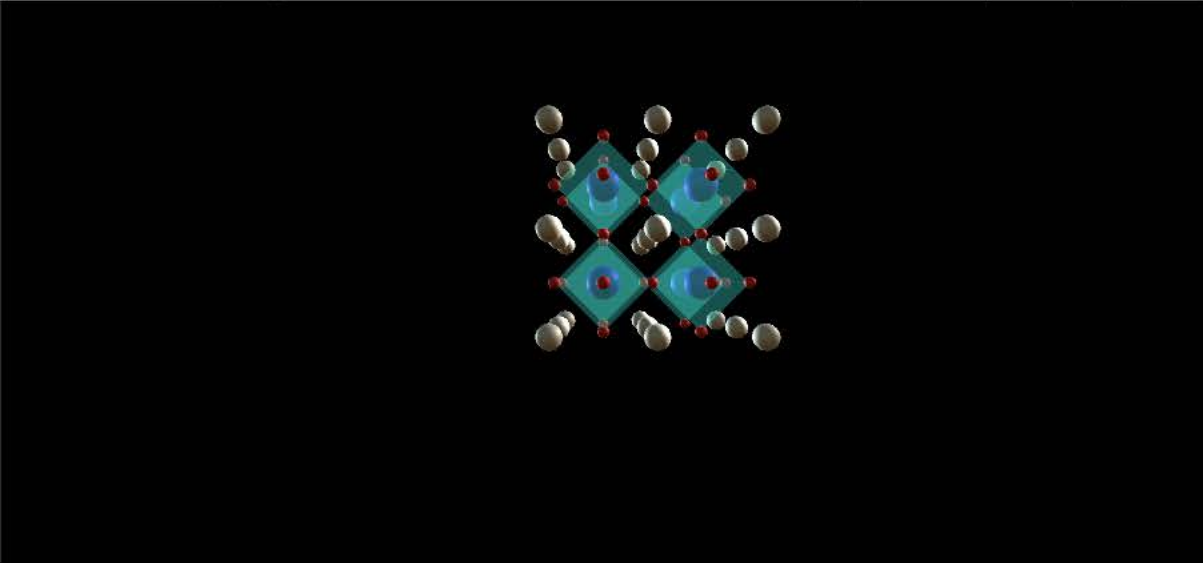
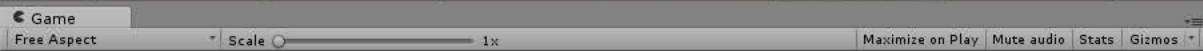
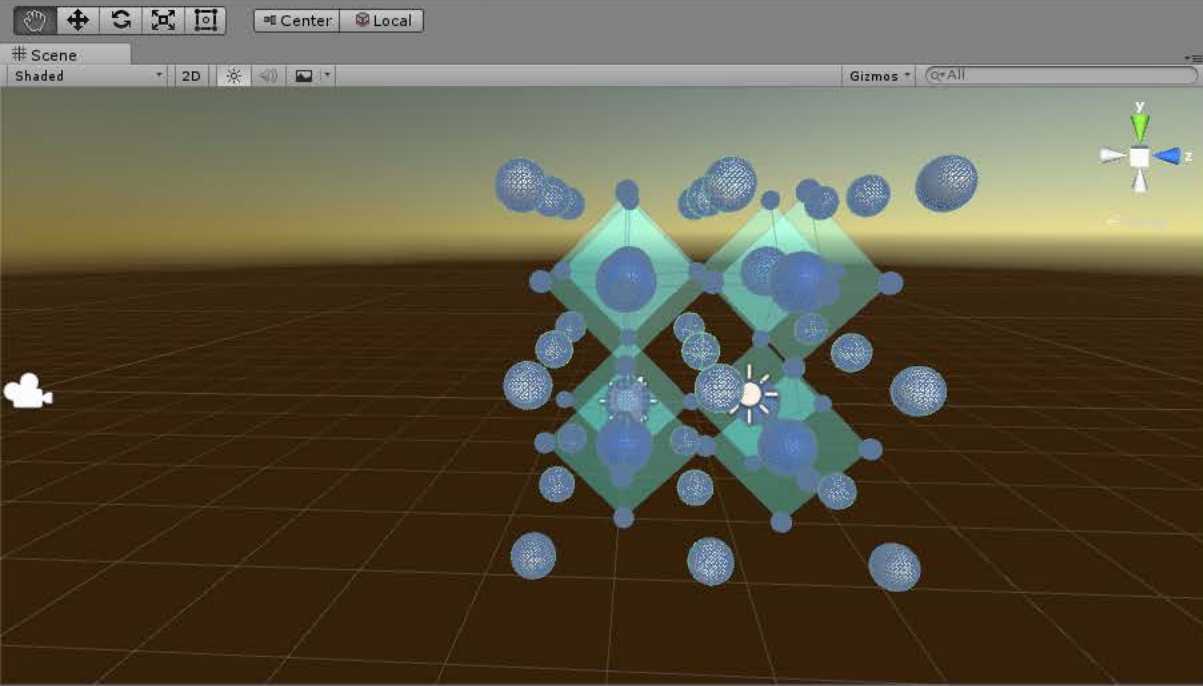
Power Button

Adjustable Wheel

Volume

Pin Demo





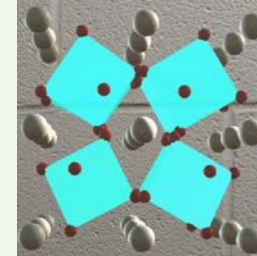
Glazer Stereophotographs

Notation

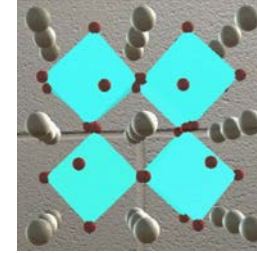
Unity App Viewed in Hololens



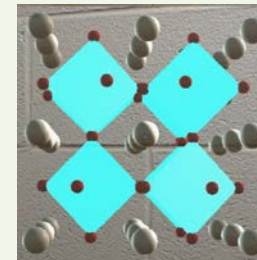
a^+, b^+, c^-



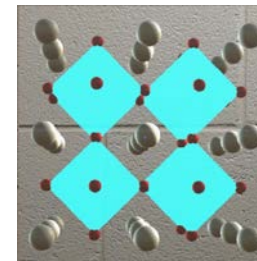
a^0, b^+, c^-



a^0, b^0, c^-



a^0, b^0, c^0







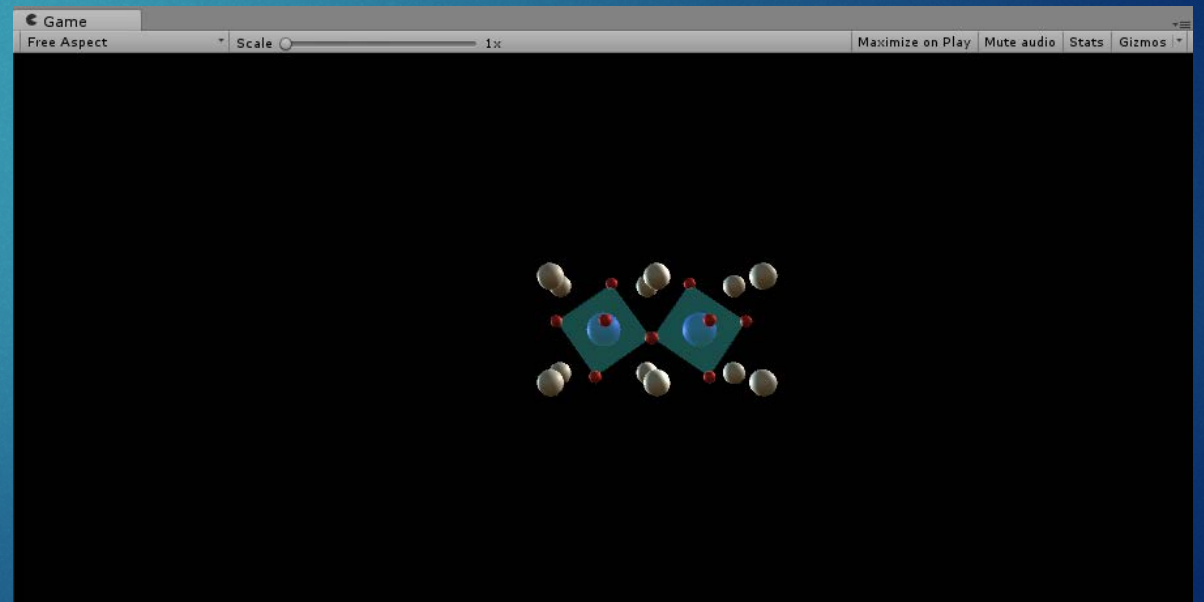
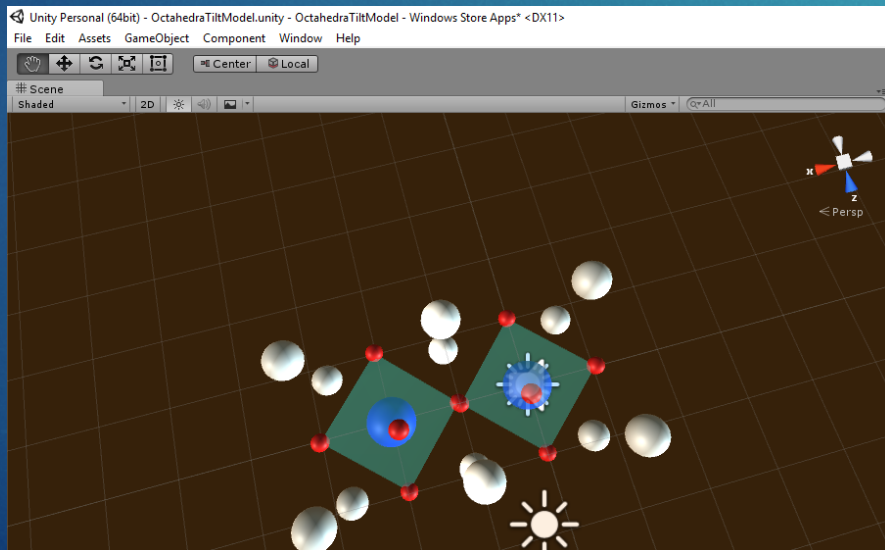
Results



- ▶ Visualize and manipulate a crystal
- ▶ Detect when crystal is being selected (audio)

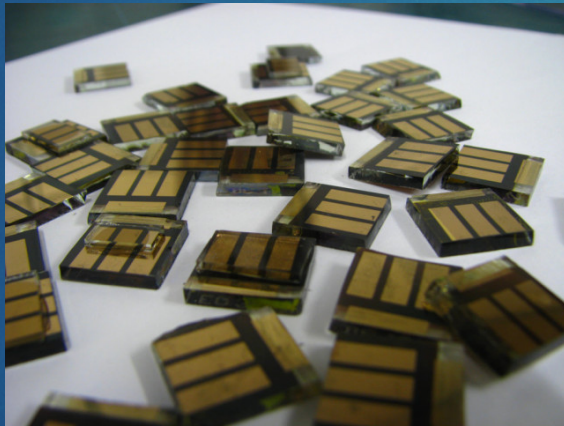
Future Goals

- ▶ Toolbar – rotation, movement, initiating “octahedral tilt”
- ▶ Voice and Spatial Recognition
- ▶ Implementation of data



Practical Applications

- ▶ Solar Cells
 - ▶ organic-inorganic semiconductors for efficient photovoltaics
- ▶ Microelectronics and Telecommunications



Courtesy of Uclia Wang



Courtesy of Tan, Moghaddam, Lai, et al.

Acknowledgements

- ▶ William Ratcliff
- ▶ Don Lopez
- ▶ NIST, NCNR
- ▶ CHRNS

